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First-principles study of electronic, magnetic, and mechanical properties in pristine and 3D-metal intercalated titanium dichalcogenides TiX_2 and $YTiX_2$ (X = S, Se, Te; Y = Cr, Mn, Fe)

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Abstract

This work presents a comprehensive first-principles investigation of the structural, electronic, magnetic, and mechanical properties of the layered titanium dichalcogenides TiX_2 (X = S, Se, Te) and their magnetically intercalated variants $YTiX_2$ (Y = Cr, Mn, Fe). All compounds are found to crystallize in the hexagonal 1T-CdI_2 structure (space group P $\bar{3}$ m1), with intercalation occurring at the octahedral site within the van der Waals gap. Our calculations reveal that while the parent TiX_2 compounds are non-magnetic semiconductors (TiS_2) or metals ($TiSe_2$, $TiTe_2$), intercalation induces a transition to ferromagnetic metallic ($CrTiX_2$, $MnTiSe_2$, $MnTiTe_2$, and $FeTiTe_2$) or half-metallic ($MnTiS_2$, $FeTiS_2$, and $FeTiSe_2$) states, the latter exhibiting 100% spin polarization at the Fermi level —a coveted property for spintronics. Magnetic moment analysis reveals complex interplay between localized moments on the intercalants and induced antiparallel moments on Ti atoms, mediated by strong superexchange coupling. Mechanically, all compounds are stable and exhibit significant anisotropy, which is visually confirmed by 3D representations of elastic moduli. The pristine compounds show classic layer-driven anisotropy ($C_{11} > C_{33}$), which is often inverted ($C_{33} > C_{11}$) upon intercalation due to a covalent 'pillaring' effect. Pugh's and Poisson's ratios classify most compounds as brittle with mixed ionic-covalent bonding, with notable exceptions like $FeTiSe_2$ and $MnTiTe_2$ showing a ductile character. This study provides a calculated foundation for experimental work by establishing the elastic stability, predicting structural parameters, and identifying the promising half-metallic ferromagnetism in $MnTiS_2$ and $FeTiS_2$, thereby guiding the targeted synthesis and characterization of these materials for spintronic applications.

1. Introduction

The pursuit of advanced functional materials has intensified research on transition metal dichalcogenides (TMDs) and their intercalation compounds, driven by their exceptional properties relevant to spintronics, quantum information processing, and solid-state thermoelectrics [1–3]. Within this class, the titanium dichalcogenide series TiX_2 (X = S, Se, Te) serves as a foundational system, crystallizing in the canonical 1T-CdI_2 prototype structure. This layered architecture features a plane of titanium atoms octahedrally coordinated by two closed-packed chalcogen layers, facilitating anisotropic physical properties and enabling host–guest chemistry via intercalation.

A longstanding and critical debate surrounds the fundamental electronic nature of the pristine TiX_2 compounds. Titanium diselenide ($TiSe_2$) exhibits a charge density wave (CDW) transition below ~220 K [4], which is often linked to its contested electronic ground state, described variably as semiconducting [5, 6] or semimetallic [7]. In contrast, TiS_2 shows no CDW instability, yet its electronic character is similarly disputed. While